Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Supporting Information

Fluorogenic Sensing of $CH_3CO_2^-$ and $H_2PO_4^-$ by Ditopic Receptor through Conformational Change

Nisar Ahmed,*[a] Vangaru Suresh,[a] Bahareh Shirinfar,[a] Inacrist Geronimo,[a] Amita Bist,[a] In-Chul Hwang,[a] and Kwang S. Kim,*[a]

[a]Center for Superfunctional Materials, Department of Chemistry

Pohang University of Science and Technology, Pohang, Korea

* E-mail: kim@postech.ac.kr, nisar@postech.ac.kr

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1. NMR Spectral Analysis

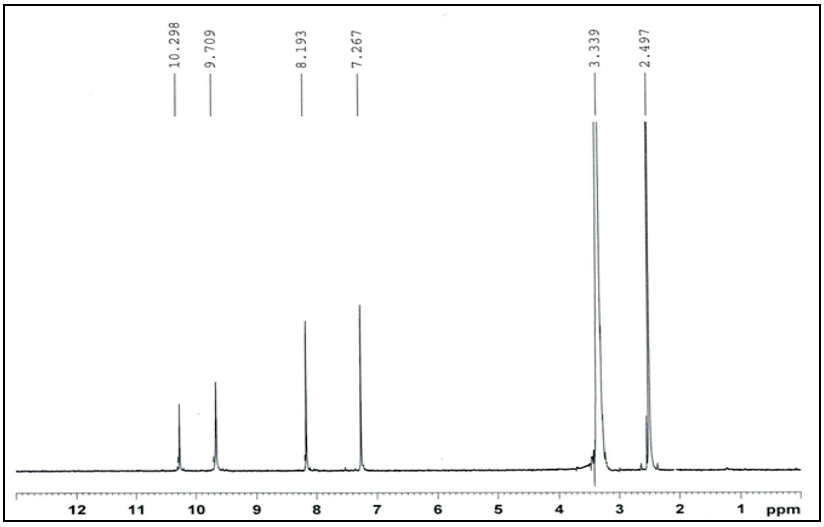

FIGURE S1. ^{1}H-NMR spectrum of compound **1** in DMSO-d_6.

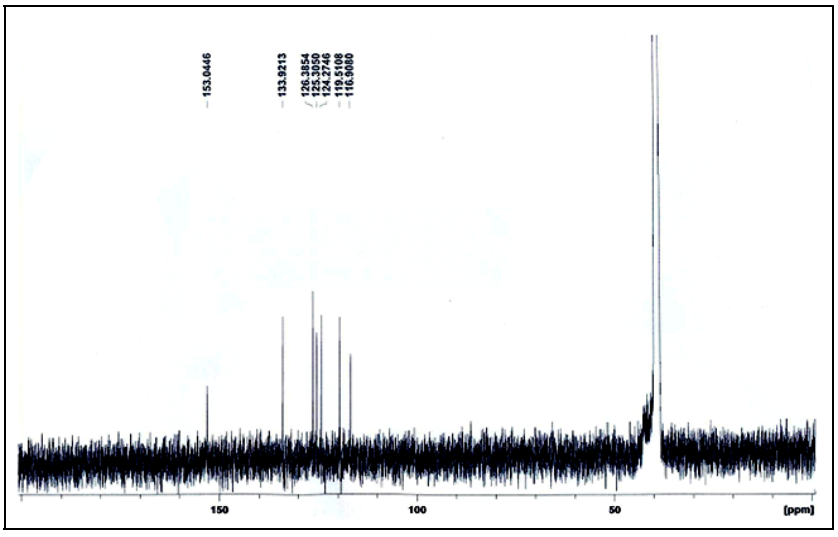

FIGURE S2. ^{13}C-NMR spectrum of compound **1** in DMSO-d_6.

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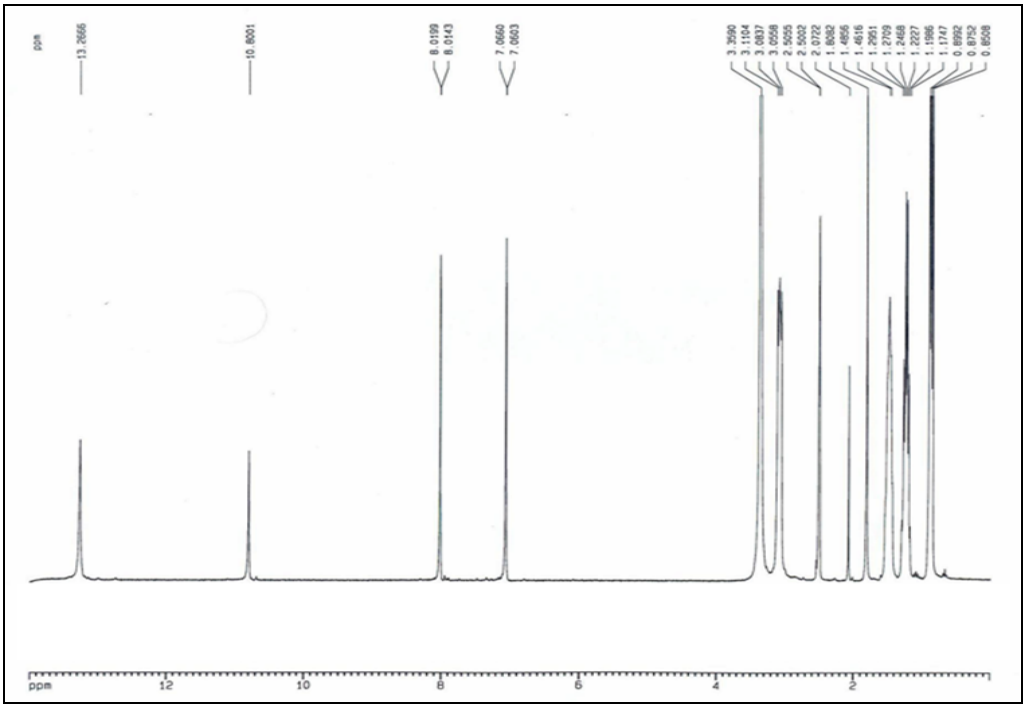

FIGURE S3. ^{1}H-NMR spectrum of compound **1**·$(CH_3CO_2^-)_2$·$(t\text{-}Bu_4N^+)_2$ in DMSO-d_6.

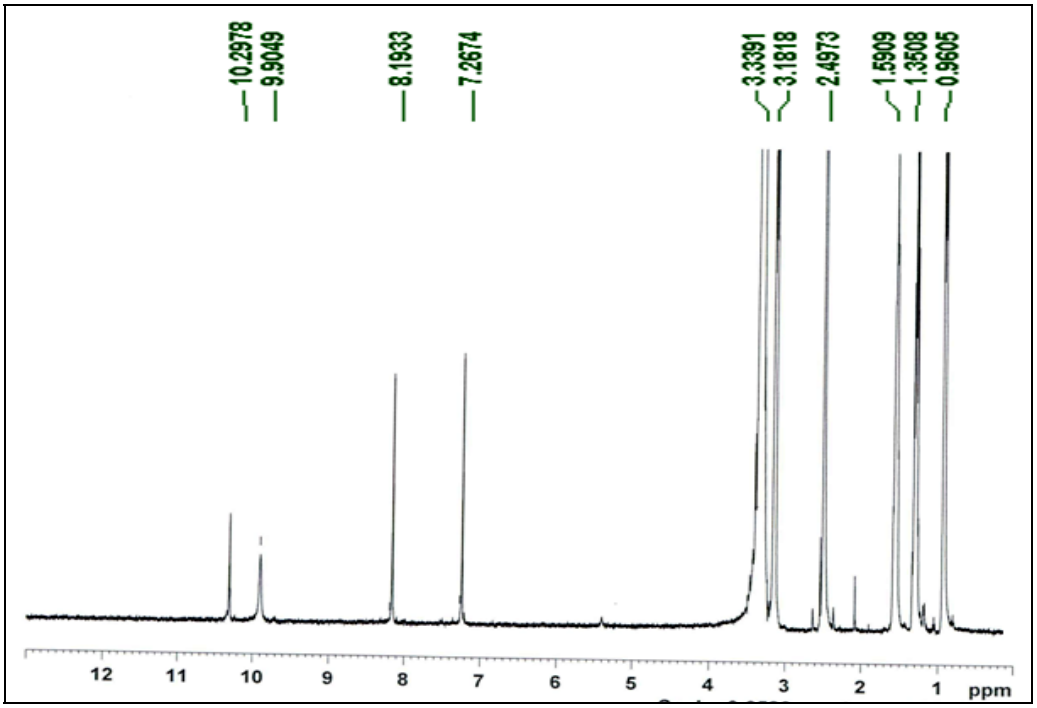

FIGURE S4. ^{1}H-NMR spectrum of compound **1**·$(Cl^-)_2$·$(t\text{-}Bu_4N^+)_2$ in DMSO-d_6.

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2. Fluorometric Analysis

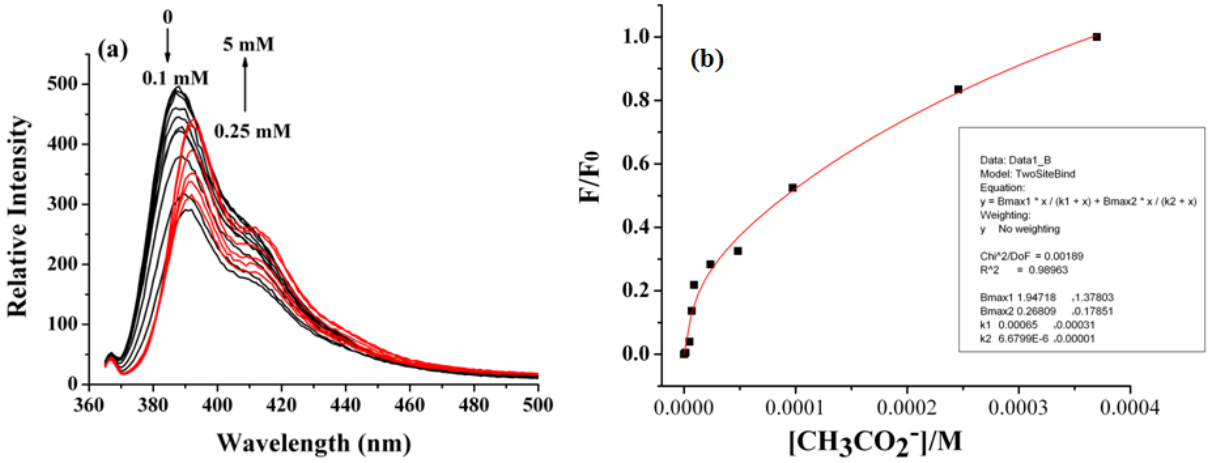

FIGURE S5. Emission spectra of **1** (10 μM) in DMSO observed during the course of the titration with $TBA^{+}CH_3CO_2^{-}$ and the corresponding binding isotherm (F and F_0 are the fluorescence signals at 387 nm in the presence and absence of $CH_3CO_2^{-}$, respectively).

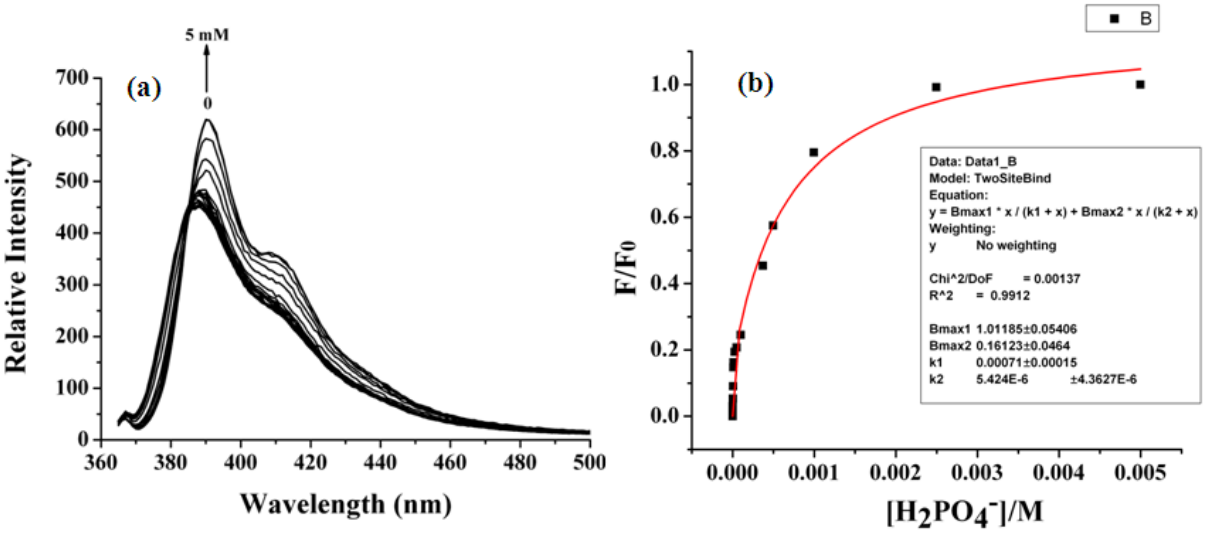

FIGURE S6. Emission spectra of **1** (10 μM) in DMSO observed during the course of the titration with $TBA^{+}H_2PO_4^{-}$ and the corresponding binding isotherm (F and F_0 are the fluorescence signals at 390 nm in the presence and absence of $H_2PO_4^{-}$, respectively).

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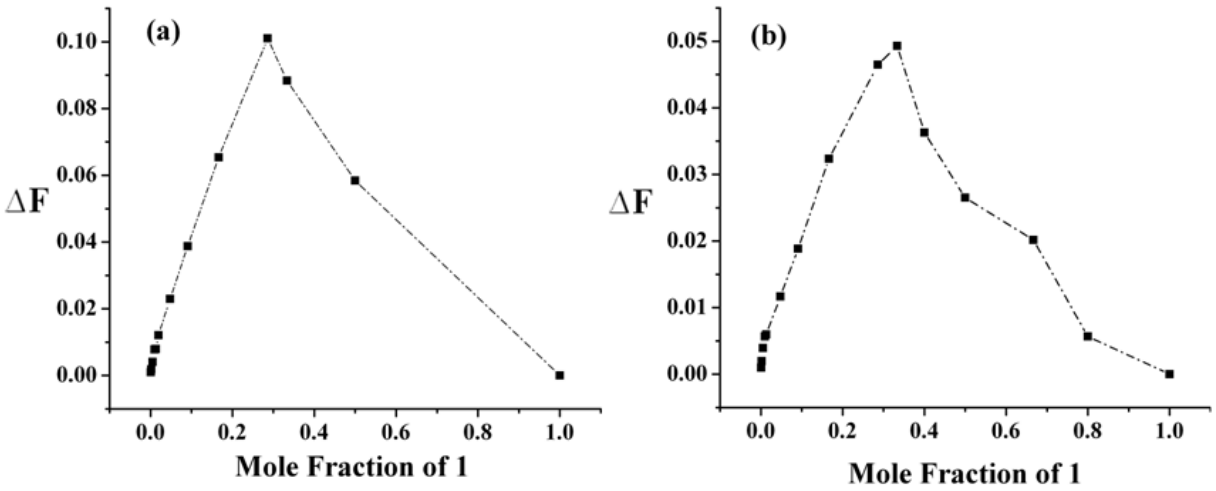

FIGURE S7. Assessment of the stoichiometry of the (a) $CH_3CO_2^-$ and (b) $H_2PO_4^-$ complexes of **1** via Job plot analysis; [1] + [anion] = 10 μM, DMSO, 25ºC.

3. Theoretical Calculations

Density functional theory (DFT) using Grimme's functional with dispersion (B97-D) and TZV2P basis set was used to optimize the $CH_3CO_2^-$ and $H_2PO_4^-$ complexes of **1**. Single point energies in DMSO solution were calculated using the integral equation formalism variant of the Polarizable Continuum Model (IEFPCM). Time-dependent DFT (TDDFT) and NMR calculations on the optimized geometries were done at the B98/TZVP and B97-D/TZV2P level, respectively. All calculations were performed using Gaussian 09.[1]

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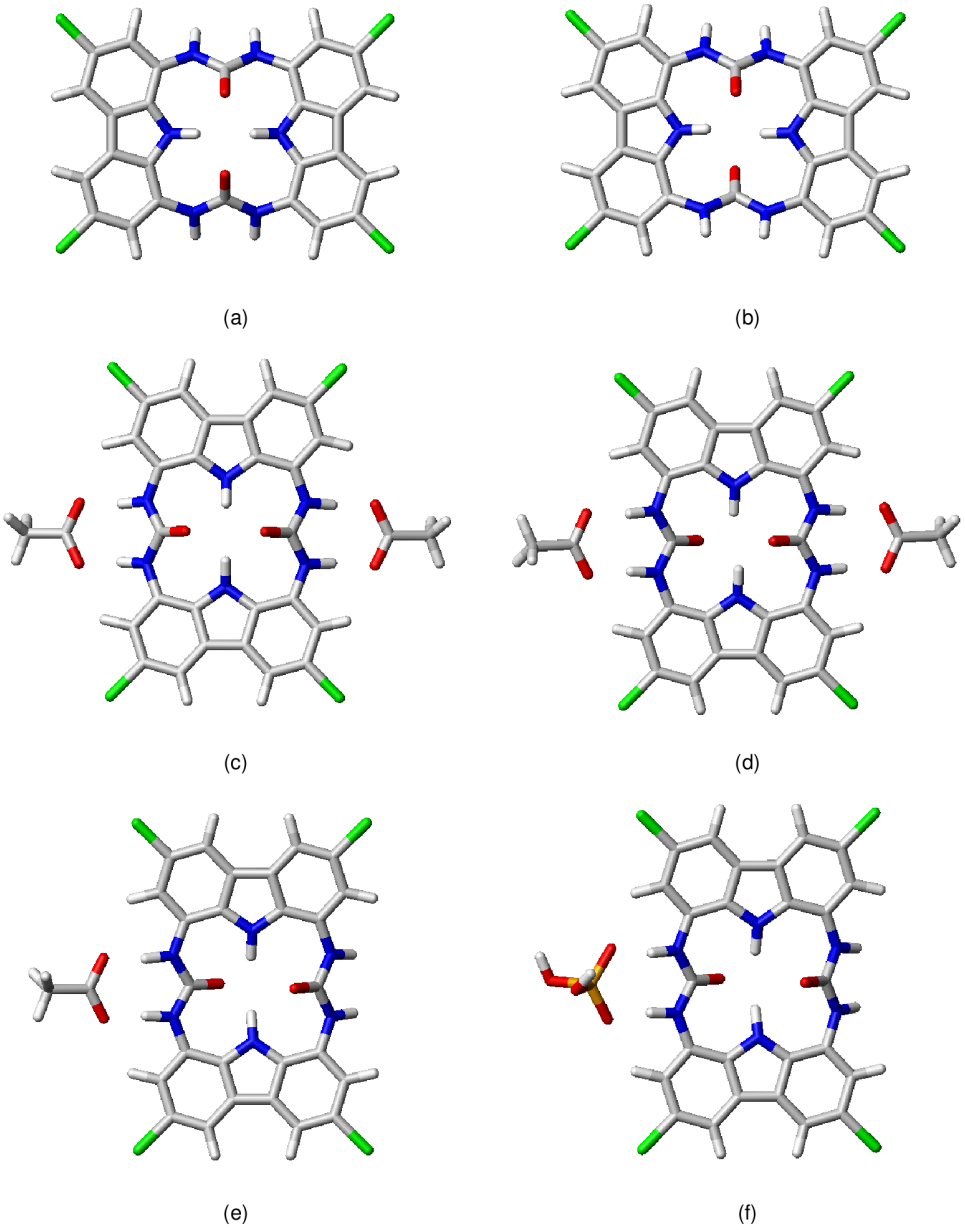

FIGURE S8. Optimized geometries calculated at the B97-D/TZV2P level of (a) cis and (b) trans conformers of **1**; (c) cis and (d) trans conformers of **1**-2·$CH_3CO_2^-$; trans conformers of 1:1 complexes with (e) $CH_3CO_2^-$ and (f) $H_2PO_4^-$.

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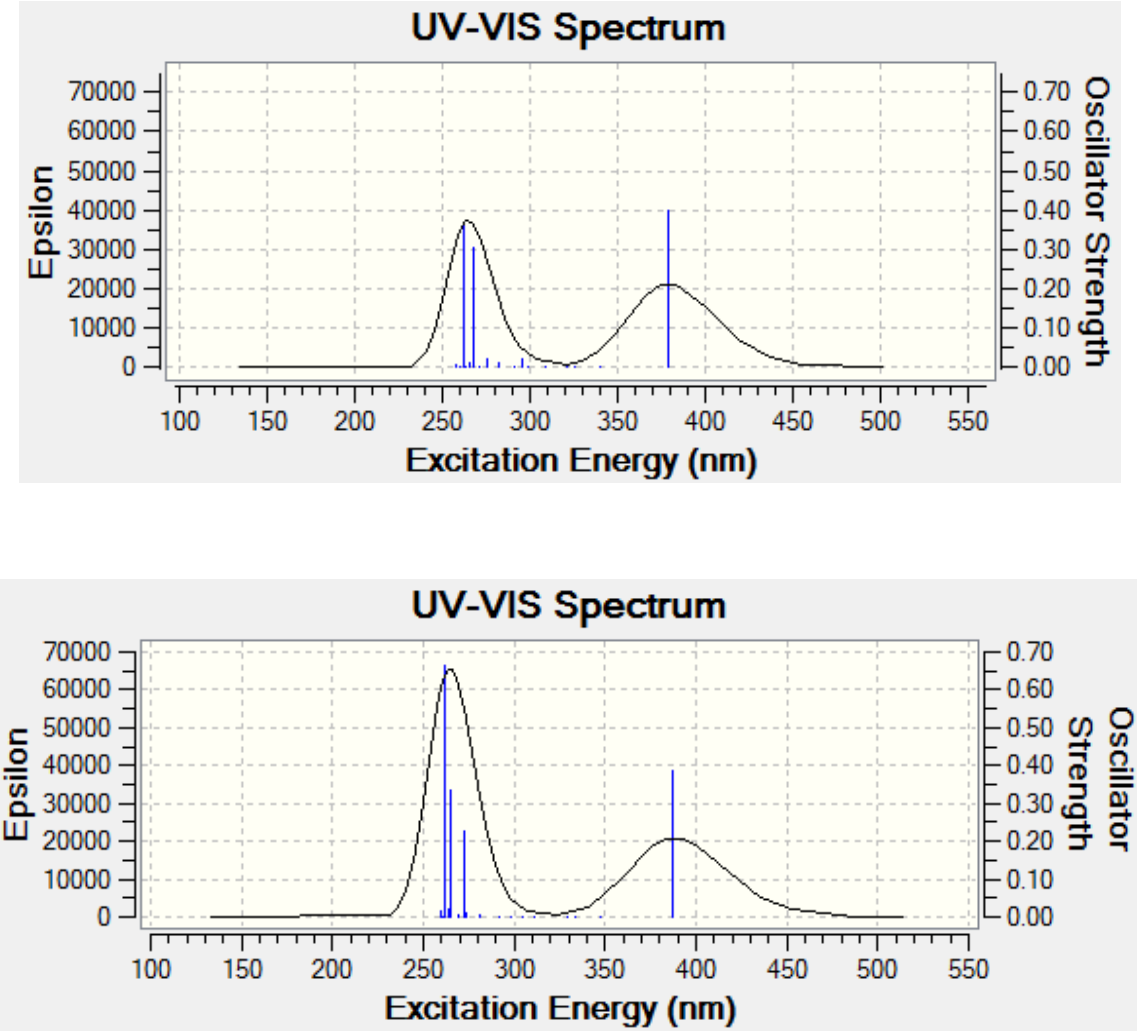

FIGURE S9. UV-Vis spectra of the cis (top) and trans (bottom) conformers of **1**-2·$CH_3CO_2^-$ obtained at the B98/TZVP level.

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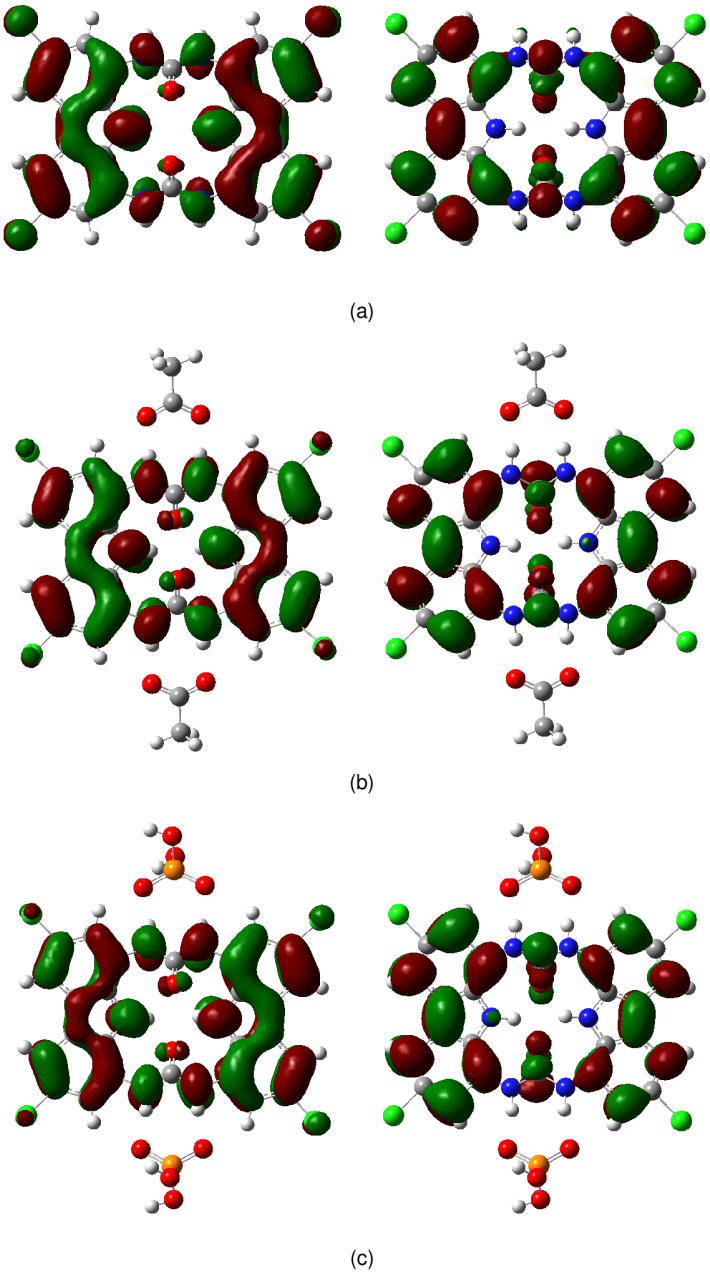

FIGURE S10. Molecular orbital representations of the highest occupied molecular orbital (HOMO) and lowest molecular orbital (LUMO) of (a) **1**, (b) trans **1**-2·$CH_3CO_2^-$ and (c) trans **1**-2·$H_2PO_4^-$.

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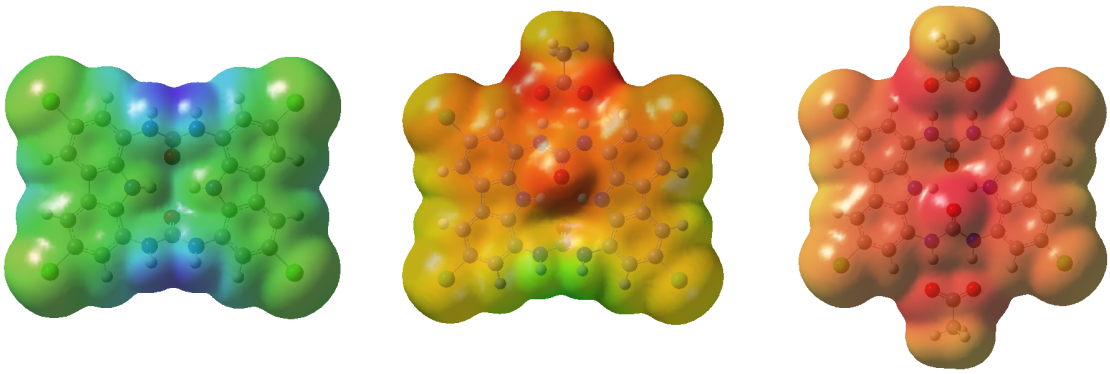

(a) (b) (c)

FIGURE S11. Molecular electrostatic potential of the (a) cis conformer of **1**, (b) trans 1:1 $CH_3CO_2^-$ complex and (c) trans 1:2 $CH_3CO_2^-$ complex. Negative potential is shown in red and positive potential in blue.

4. X-ray Crystallographic Data

TABLE S1. Crystal data and structure refinement for **1**·2[$(n\text{-Bu})_4N^+\cdot(CH_3CO_2)^-$]

Empirical formula	$C_{62}\ H_{90}\ Cl_4\ N_8\ O_2$
Formula weight	1185.22
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P21/n
Unit cell dimensions	a = 8.8875(11) Å α = 64.753(2)°
	b = 13.7511(17) Å β = 77.356(3)°
	c = 15.0665(19) Å γ = 74.412(2)°
Volume	1592.6(3) $Å^3$
Z	1
Density (calculated)	1.235 Mg/m^3
Absorption coefficient	0.241 mm^{-1}
F(000)	634
Theta range for data collection	1.51 to 25.07°.
Index ranges	-10<=h<=9, -16<=k<=16, -13<=l<=18
Reflections collected	8908
Independent reflections	5938 [R(int) = 0.0212]
Completeness to theta = 25.11°	97.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5938 / 0 / 366
Goodness-of-fit on F^2	1.089
Final R indices [I>2sigma(I)]	R1 = 0.0641, wR2 = 0.1584
R indices (all data)	R1 = 0.1184, wR2 = 0.2103
Largest diff. peak and hole	0.318 and -0.229 $e.Å^{-3}$

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TABLE S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1**·2[(*n*-Bu)$_4$N$^+$·(CH$_3$CO$_2$)$^-$]·2DMSO. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	X	y	z	U(eq)
Cl(1)	-393(1)	8902(1)	12024(1)	93(1)
Cl(2)	5926(2)	10628(1)	6731(1)	116(1)
O(1)	6920(2)	5275(2)	9522(2)	53(1)
N(1)	4092(3)	6620(2)	9748(2)	50(1)
N(2)	6458(3)	6501(2)	7956(2)	51(1)
N(3)	7573(3)	4712(2)	8232(2)	55(1)
C(1)	2983(4)	7012(2)	10360(3)	49(1)
C(2)	2827(4)	8158(2)	9997(3)	53(1)
C(3)	1783(4)	8760(3)	10502(3)	63(1)
C(4)	930(4)	8195(3)	11358(3)	61(1)
C(5)	4698(4)	7465(2)	8985(3)	48(1)
C(6)	3938(4)	8448(3)	9110(3)	54(1)
C(7)	4327(4)	9443(3)	8408(3)	64(1)
C(8)	5402(5)	9415(3)	7625(3)	66(1)
C(9)	6138(4)	8442(3)	7483(3)	60(1)
C(10)	5803(4)	7442(2)	8164(3)	48(1)
C(11)	6973(4)	5480(3)	8638(3)	47(1)
C(12)	2136(4)	6437(2)	11265(3)	49(1)
C(13)	1099(4)	7055(3)	11740(3)	57(1)
N(4)	8066(3)	3365(2)	2911(2)	53(1)
C(14)	6905(4)	4415(3)	2436(3)	57(1)
C(15)	7424(4)	5478(3)	2192(3)	65(1)
C(16)	6283(4)	6451(3)	1580(3)	69(1)
C(17)	6526(5)	7551(3)	1492(3)	87(1)
C(18)	8554(4)	3354(3)	3812(3)	60(1)
C(19)	7236(4)	3447(3)	4618(3)	69(1)
C(20)	7838(5)	3285(3)	5534(3)	78(1)
C(21)	6547(5)	3462(4)	6314(3)	93(1)
C(22)	7243(4)	2417(3)	3191(3)	58(1)
C(23)	8143(4)	1287(3)	3774(3)	73(1)
C(24)	7263(5)	413(3)	4008(4)	88(1)
C(25)	8125(6)	-721(3)	4604(4)	113(2)
C(26)	9535(4)	3266(3)	2191(3)	60(1)
C(27)	10691(4)	2889(3)	663(3)	76(1)
C(28)	9280(4)	3392(4)	1188(3)	79(1)
C(29)	10977(6)	1650(4)	1076(4)	105(2)
C(30)	2404(4)	3807(3)	4276(3)	59(1)
C(31)	2238(5)	3587(3)	5359(3)	80(1)
O(2)	1413(3)	4557(2)	3757(2)	75(1)
O(3)	3530(3)	3239(2)	3950(2)	81(1)

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TABLE S3. Bond lengths [Å] and angles [°] for **1**·2[(n-Bu)$_4$N$^+$·(CH$_3$CO$_2$)$^-$]·2DMSO.

Cl(1)-C(4)	1.743(4)	C(1)-N(1)-C(5)	110.2(3)	C(18)-C(19)-H(19B)	109.2
Cl(2)-C(8)	1.743(4)	C(1)-N(1)-H(1)	124.9	H(19A)-C(19)-H(19B)	107.9
O(1)-C(11)	1.232(4)	C(5)-N(1)-H(1)	124.9	C(19)-C(20)-C(21)	113.0(3)
N(1)-C(1)	1.361(4)	C(11)-N(2)-C(10)	125.0(3)	C(19)-C(20)-H(20A)	109.0
N(1)-C(5)	1.374(4)	C(11)-N(2)-H(2)	117.5	C(21)-C(20)-H(20A)	109.0
N(1)-H(1)	0.860	C(10)-N(2)-H(2)	117.5	C(19)-C(20)-H(20B)	109.0
N(2)-C(11)	1.366(4)	C(11)-N(3)-C(12)#1	127.2(3)	C(21)-C(20)-H(20B)	109.0
N(2)-C(10)	1.405(4)	C(11)-N(3)-H(3N)	116.4	H(20A)-C(20)-H(20B)	107.8
N(2)-H(2)	0.860	C(12)#1-N(3)-H(3N)	116.4	C(20)-C(21)-H(21A)	109.5
N(3)-C(11)	1.371(4)	N(1)-C(1)-C(2)	109.1(3)	C(20)-C(21)-H(21B)	109.5
N(3)-C(12)#1	1.408(4)	N(1)-C(1)-C(12)	129.7(3)	H(21A)-C(21)-H(21B)	109.5
N(3)-H(3N)	0.860	C(2)-C(1)-C(12)	121.0(3)	C(20)-C(21)-H(21C)	109.5
C(1)-C(2)	1.408(4)	C(3)-C(2)-C(1)	120.7(3)	H(21A)-C(21)-H(21C)	109.5
C(1)-C(12)	1.415(5)	C(3)-C(2)-C(6)	133.4(3)	H(21B)-C(21)-H(21C)	109.5
C(2)-C(3)	1.394(5)	C(1)-C(2)-C(6)	105.9(3)	C(23)-C(22)-N(4)	115.7(3)
C(2)-C(6)	1.450(5)	C(4)-C(3)-C(2)	117.5(3)	C(23)-C(22)-H(22A)	108.4
C(3)-C(4)	1.369(5)	C(4)-C(3)-H(3)	121.3	N(4)-C(22)-H(22A)	108.4
C(3)-H(3)	0.930	C(2)-C(3)-H(3)	121.3	C(23)-C(22)-H(22B)	108.4
C(4)-C(13)	1.397(4)	C(3)-C(4)-C(13)	122.6(3)	N(4)-C(22)-H(22B)	108.4
C(5)-C(10)	1.406(5)	C(3)-C(4)-Cl(1)	119.6(3)	H(22A)-C(22)-H(22B)	107.4
C(5)-C(6)	1.412(4)	C(13)-C(4)-Cl(1)	117.8(3)	C(24)-C(23)-C(22)	112.1(3)
C(6)-C(7)	1.403(4)	N(1)-C(5)-C(10)	129.4(3)	C(24)-C(23)-H(23A)	109.2
C(7)-C(8)	1.354(5)	N(1)-C(5)-C(6)	107.9(3)	C(22)-C(23)-H(23A)	109.2
C(7)-H(7)	0.930	C(10)-C(5)-C(6)	122.5(3)	C(24)-C(23)-H(23B)	109.2
C(8)-C(9)	1.405(5)	C(7)-C(6)-C(5)	119.2(3)	C(22)-C(23)-H(23B)	109.2
C(9)-C(10)	1.384(4)	C(7)-C(6)-C(2)	134.0(3)	H(23A)-C(23)-H(23B)	107.9
C(9)-H(9)	0.930	C(5)-C(6)-C(2)	106.8(3)	C(23)-C(24)-C(25)	113.2(4)
C(12)-C(13)	1.376(4)	C(8)-C(7)-C(6)	118.0(3)	C(23)-C(24)-H(24A)	108.9
C(12)-N(3)#1	1.408(4)	C(8)-C(7)-H(7)	121.0	C(25)-C(24)-H(24A)	108.9
C(13)-H(13)	0.930	C(6)-C(7)-H(7)	121.0	C(23)-C(24)-H(24B)	108.9
N(4)-C(18)	1.507(4)	C(7)-C(8)-C(9)	123.2(3)	C(25)-C(24)-H(24B)	108.9
N(4)-C(14)	1.518(4)	C(7)-C(8)-Cl(2)	119.8(3)	H(24A)-C(24)-H(24B)	107.8
N(4)-C(26)	1.520(4)	C(9)-C(8)-Cl(2)	117.0(3)	C(24)-C(25)-H(25A)	109.5
N(4)-C(22)	1.522(4)	C(10)-C(9)-C(8)	120.7(4)	C(24)-C(25)-H(25B)	109.5
C(14)-C(15)	1.522(4)	C(10)-C(9)-H(9)	119.7	H(25A)-C(25)-H(25B)	109.5
C(14)-H(14A)	0.970	C(8)-C(9)-H(9)	119.7	C(24)-C(25)-H(25C)	109.5
C(14)-H(14B)	0.970	C(9)-C(10)-N(2)	119.0(3)	H(25A)-C(25)-H(25C)	109.5
C(15)-C(16)	1.515(4)	C(9)-C(10)-C(5)	116.4(3)	H(25B)-C(25)-H(25C)	109.5
C(15)-H(15A)	0.970	N(2)-C(10)-C(5)	124.3(3)	C(28)-C(26)-N(4)	116.4(3)
C(15)-H(15B)	0.970	O(1)-C(11)-N(2)	123.5(3)	C(28)-C(26)-H(26A)	108.2
C(16)-C(17)	1.531(5)	O(1)-C(11)-N(3)	123.6(3)	N(4)-C(26)-H(26A)	108.2
C(16)-H(16A)	0.970	N(2)-C(11)-N(3)	112.9(3)	C(28)-C(26)-H(26B)	108.2
C(16)-H(16B)	0.970	C(13)-C(12)-N(3)#1	117.9(3)	N(4)-C(26)-H(26B)	108.2
C(17)-H(17A)	0.960	C(13)-C(12)-C(1)	117.0(3)	H(26A)-C(26)-H(26B)	107.3
C(17)-H(17B)	0.960	N(3)#1-C(12)-C(1)	124.5(3)	C(28)-C(27)-C(29)	113.5(4)
C(17)-H(17C)	0.960	C(12)-C(13)-C(4)	121.3(3)	C(28)-C(27)-H(27A)	108.9
C(18)-C(19)	1.513(5)	C(12)-C(13)-H(13)	119.4	C(29)-C(27)-H(27A)	108.9
C(18)-H(18A)	0.970	C(4)-C(13)-H(13)	119.4	C(28)-C(27)-H(27B)	108.9
C(18)-H(18B)	0.970	C(18)-N(4)-C(14)	110.5(3)	C(29)-C(27)-H(27B)	108.9
C(19)-C(20)	1.496(5)	C(18)-N(4)-C(26)	108.1(2)	H(27A)-C(27)-H(27B)	107.7
C(19)-H(19A)	0.970	C(14)-N(4)-C(26)	110.5(3)	C(27)-C(28)-C(26)	113.6(3)

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C(19)-H(19B)	0.970	C(18)-N(4)-C(22)	110.7(3)	C(27)-C(28)-H(28A)	108.8
C(20)-C(21)	1.503(5)	C(14)-N(4)-C(22)	107.0(2)	C(26)-C(28)-H(28A)	108.8
C(20)-H(20A)	0.970	C(26)-N(4)-C(22)	110.0(3)	C(27)-C(28)-H(28B)	108.8
C(20)-H(20B)	0.970	N(4)-C(14)-C(15)	116.0(3)	C(26)-C(28)-H(28B)	108.8
C(21)-H(21A)	0.960	N(4)-C(14)-H(14A)	108.3	H(28A)-C(28)-H(28B)	107.7
C(21)-H(21B)	0.960	C(15)-C(14)-H(14A)	108.3	C(27)-C(29)-H(29A)	109.5
C(21)-H(21C)	0.960	N(4)-C(14)-H(14B)	108.3	C(27)-C(29)-H(29B)	109.5
C(22)-C(23)	1.517(4)	C(15)-C(14)-H(14B)	108.3	H(29A)-C(29)-H(29B)	109.5
C(22)-H(22A)	0.970	H(14A)-C(14)-H(14B)	107.4	C(27)-C(29)-H(29C)	109.5
C(22)-H(22B)	0.970	C(16)-C(15)-C(14)	110.3(3)	H(29A)-C(29)-H(29C)	109.5
C(23)-C(24)	1.485(5)	C(16)-C(15)-H(15A)	109.6	H(29B)-C(29)-H(29C)	109.5
C(23)-H(23A)	0.970	C(14)-C(15)-H(15A)	109.6	O(3)-C(30)-O(2)	124.0(4)
C(23)-H(23B)	0.970	C(16)-C(15)-H(15B)	109.6	O(3)-C(30)-C(31)	117.7(4)
C(24)-C(25)	1.513(6)	C(14)-C(15)-H(15B)	109.6	O(2)-C(30)-C(31)	118.3(4)
C(24)-H(24A)	0.970	H(15A)-C(15)-H(15B)	108.1	C(30)-C(31)-H(31A)	109.5
C(24)-H(24B)	0.970	C(15)-C(16)-C(17)	113.0(3)	C(30)-C(31)-H(31B)	109.5
C(25)-H(25A)	0.960	C(15)-C(16)-H(16A)	109.0	H(31A)-C(31)-H(31B)	109.5
C(25)-H(25B)	0.960	C(17)-C(16)-H(16A)	109.0	C(30)-C(31)-H(31C)	109.5
C(25)-H(25C)	0.960	C(15)-C(16)-H(16B)	109.0	H(31A)-C(31)-H(31C)	109.5
C(26)-C(28)	1.507(5)	C(17)-C(16)-H(16B)	109.0	H(31B)-C(31)-H(31C)	109.5
C(26)-H(26A)	0.970	H(16A)-C(16)-H(16B)	107.8		
C(26)-H(26B)	0.970	C(16)-C(17)-H(17A)	109.5		
C(27)-C(28)	1.498(5)	C(16)-C(17)-H(17B)	109.5		
C(27)-C(29)	1.512(5)	H(17A)-C(17)-H(17B)	109.5		
C(27)-H(27A)	0.970	C(16)-C(17)-H(17C)	109.5		
C(27)-H(27B)	0.970	H(17A)-C(17)-H(17C)	109.5		
C(28)-H(28A)	0.970	H(17B)-C(17)-H(17C)	109.5		
C(28)-H(28B)	0.970	N(4)-C(18)-C(19)	115.7(3)		
C(29)-H(29A)	0.960	N(4)-C(18)-H(18A)	108.3		
C(29)-H(29B)	0.960	C(19)-C(18)-H(18A)	108.3		
C(29)-H(29C)	0.960	N(4)-C(18)-H(18B)	108.3		
C(30)-O(3)	1.243(4)	C(19)-C(18)-H(18B)	108.3		
C(30)-O(2)	1.255(4)	H(18A)-C(18)-H(18B)	107.4		
C(30)-C(31)	1.508(5)	C(20)-C(19)-C(18)	112.2(3)		
C(31)-H(31A)	0.960	C(20)-C(19)-H(19A)	109.2		
C(31)-H(31B)	0.960	C(18)-C(19)-H(19A)	109.2		
C(31)-H(31C)	0.960	C(20)-C(19)-H(19B)	109.2		

TABLE S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **1**·2[(*n*-Bu)$_4$N$^+$·(CH$_3$CO$_2$)$^-$]·2DMSO. The anisotropic displacement factor exponent takes the form $-2\pi^2$ [$h^2a^{*2}U^{11}$ + … $2hka^*b^*U^{12}$].

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	105(1)	67(1)	94(1)	-44(1)	12(1)	4(1)
Cl(2)	155(1)	51(1)	112(1)	-17(1)	30(1)	-33(1)
O(1)	57(1)	46(1)	55(2)	-19(1)	-15(1)	-7(1)
N(1)	53(2)	36(1)	61(2)	-19(1)	-6(1)	-8(1)
N(2)	56(2)	42(2)	52(2)	-19(1)	-5(1)	-8(1)
N(3)	60(2)	42(2)	55(2)	-17(1)	-3(1)	-5(1)
C(1)	48(2)	43(2)	59(2)	-24(2)	-13(2)	-3(1)
C(2)	57(2)	42(2)	60(2)	-22(2)	-14(2)	-2(2)
C(3)	73(2)	41(2)	71(3)	-22(2)	-15(2)	2(2)

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C(4)	62(2)	49(2)	68(3)	-27(2)	-9(2)	3(2)
C(5)	52(2)	37(2)	57(2)	-17(2)	-16(2)	-6(1)
C(6)	57(2)	44(2)	62(2)	-19(2)	-16(2)	-6(2)
C(7)	72(2)	40(2)	78(3)	-23(2)	-11(2)	-5(2)
C(8)	80(3)	40(2)	69(3)	-14(2)	-11(2)	-11(2)
C(9)	64(2)	48(2)	62(2)	-13(2)	-8(2)	-13(2)
C(10)	46(2)	45(2)	54(2)	-19(2)	-9(2)	-6(1)
C(11)	40(2)	45(2)	58(2)	-19(2)	-6(2)	-12(1)
C(12)	47(2)	45(2)	56(2)	-20(2)	-11(2)	-3(1)
C(13)	56(2)	55(2)	57(2)	-22(2)	-7(2)	-6(2)
N(4)	44(2)	59(2)	54(2)	-19(1)	-9(1)	-10(1)
C(14)	46(2)	61(2)	62(2)	-22(2)	-12(2)	-7(2)
C(15)	63(2)	64(2)	66(3)	-22(2)	-13(2)	-14(2)
C(16)	69(2)	67(2)	67(3)	-25(2)	-13(2)	-4(2)
C(17)	100(3)	64(3)	92(3)	-31(2)	-9(3)	-10(2)
C(18)	55(2)	63(2)	61(2)	-21(2)	-16(2)	-10(2)
C(19)	68(2)	81(3)	62(2)	-31(2)	-6(2)	-19(2)
C(20)	78(3)	90(3)	71(3)	-37(2)	-15(2)	-11(2)
C(21)	89(3)	128(4)	80(3)	-55(3)	-1(3)	-34(3)
C(22)	53(2)	60(2)	63(2)	-24(2)	-6(2)	-17(2)
C(23)	66(2)	61(2)	80(3)	-16(2)	-8(2)	-15(2)
C(24)	104(3)	70(3)	98(4)	-29(3)	-27(3)	-22(2)
C(25)	149(5)	57(3)	119(4)	-24(3)	-13(4)	-18(3)
C(26)	48(2)	70(2)	60(2)	-24(2)	-5(2)	-11(2)
C(27)	69(3)	102(3)	66(3)	-39(3)	-4(2)	-21(2)
C(28)	64(3)	103(3)	59(3)	-25(2)	-9(2)	-10(2)
C(29)	135(4)	87(3)	108(4)	-45(3)	-30(4)	-21(3)
C(30)	57(2)	61(2)	60(2)	-25(2)	6(2)	-21(2)
C(31)	84(3)	88(3)	65(3)	-33(2)	-5(2)	-14(2)
O(2)	73(2)	73(2)	67(2)	-25(2)	-1(2)	-8(1)
O(3)	76(2)	90(2)	64(2)	-33(2)	-5(2)	6(2)

TABLE S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **1**·2[(*n*-Bu)$_4$N$^+$·(CH$_3$CO$_2$)$^-$]·2DMSO. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
H(1)	4374	5942	9828	60
H(2)	6540	6573	7352	61
H(3N)	7797	4959	7599	66
H(3)	1670	9518	10268	76
H(7)	3859	10102	8478	77
H(9)	6858	8471	6926	72
H(13)	500	6707	12328	69
H(14A)	5928	4401	2877	68
H(14B)	6684	4422	1831	68
H(15A)	7469	5549	2799	77
H(15B)	8469	5465	1827	77
H(16A)	5217	6369	1878	83
H(16B)	6405	6455	923	83
H(17A)	6385	7560	2139	131
H(17B)	5774	8136	1100	131
H(17C)	7571	7647	1183	131

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H(18A)	9095	3955	3604	72
H(18B)	9303	2677	4092	72
H(19A)	6559	4165	4375	82
H(19B)	6610	2902	4778	82
H(20A)	8534	3791	5361	93
H(20B)	8449	2546	5803	93
H(21A)	5974	4205	6065	139
H(21B)	6996	3324	6890	139
H(21C)	5847	2969	6483	139
H(22A)	6241	2552	3576	69
H(22B)	7023	2414	2589	69
H(23A)	9147	1141	3395	87
H(23B)	8352	1275	4385	87
H(24A)	7067	423	3396	106
H(24B)	6252	570	4376	106
H(25A)	9106	-897	4232	170
H(25B)	7492	-1248	4746	170
H(25C)	8323	-738	5212	170
H(26A)	10111	3816	2099	72
H(26B)	10197	2553	2494	72
H(27A)	11612	3110	706	91
H(27B)	10554	3172	-30	91
H(28A)	8405	3055	1265	95
H(28B)	8993	4167	782	95
H(29A)	11010	1365	1776	158
H(29B)	11961	1374	766	158
H(29C)	10141	1425	948	158
H(31A)	3147	3722	5501	120
H(31B)	2148	2837	5746	120
H(31C)	1313	4063	5520	120
H(1)	4374	5942	9828	60

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TABLE S6. Crystal data and structure refinement for **1**·2[(*n*-Bu)$_4$N$^+$·Cl$^-$].

Empirical formula	C_{58} H_{86} Cl_6 N_8 O_2
Formula weight	1140.05
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P21/n
Unit cell dimensions	a = 13.644(3) Å α = 84.368(4)°
	b = 15.163(3) Å β = 78.777(4)°
	c = 16.546(4) Å γ = 72.600(4)°
Volume	3201.2(12) Å^3
Z	2
Density (calculated)	1.183 Mg/m^3
Absorption coefficient	0.313 mm^{-1}
F(000)	1216
Theta range for data collection	1.26 to 25.11°.
Index ranges	-16<=h<=14, -18<=k<=18, -19<=l<=18
Reflections collected	16799
Independent reflections	11123 [R(int) = 0.0401]
Completeness to theta = 25.11°	97.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11123 / 0 / 675
Goodness-of-fit on F^2	0.955
Final R indices [I>2sigma(I)]	R1 = 0.0773, wR2 = 0.1903
R indices (all data)	R1 = 0.2370, wR2 = 0.2824
Largest diff. peak and hole	0.286 and -0.222 e.Å^{-3}

TABLE S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1**·2[(*n*-Bu)$_4$N$^+$·Cl$^-$]·2DMSO. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	-2329(5)	8245(4)	3712(5)	77(2)
C(2)	-1949(6)	8135(4)	4456(5)	79(2)
C(3)	-2680(6)	8299(4)	5163(4)	88(2)
C(4)	-3743(6)	8569(5)	5134(5)	98(2)
C(5)	-4141(5)	8672(4)	4432(5)	100(2)
C(6)	-3406(5)	8509(4)	3692(5)	84(2)
C(7)	-3513(5)	8512(4)	2840(5)	84(2)
C(8)	-4364(5)	8663(5)	2454(5)	100(2)
C(9)	-4179(5)	8571(5)	1622(6)	97(2)
C(10)	-3179(6)	8336(4)	1153(4)	90(2)
C(11)	-2317(5)	8172(4)	1528(5)	79(2)
C(12)	-2501(5)	8266(4)	2386(4)	76(2)
C(13)	-403(5)	7966(5)	1158(4)	78(2)
C(14)	1870(5)	7304(4)	1455(5)	78(2)
C(15)	1501(5)	7327(4)	700(5)	80(2)
C(16)	2229(6)	7134(4)	-3(5)	93(2)
C(17)	3282(7)	6929(5)	8(5)	104(2)

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C(18)	3652(5)	6908(5)	735(6)	104(2)
C(19)	2950(5)	7107(4)	1472(5)	89(2)
C(20)	3055(6)	7111(4)	2315(5)	87(2)
C(21)	3913(5)	6947(5)	2716(6)	105(2)
C(22)	3717(6)	6979(5)	3548(6)	105(2)
C(23)	2714(6)	7136(4)	4015(5)	98(2)
C(24)	1853(5)	7311(4)	3637(5)	81(2)
C(25)	2040(5)	7293(4)	2782(5)	83(2)
C(26)	-65(5)	7925(5)	3961(5)	77(2)
C(27)	9189(7)	4720(5)	2347(5)	132(3)
C(28)	9846(11)	5376(8)	2101(7)	225(6)
C(29)	11027(12)	4819(14)	2038(10)	305(12)
C(30)	11559(16)	4837(14)	2476(12)	402(16)
C(31)	7583(8)	5700(6)	1840(7)	158(3)
C(32)	7696(10)	5179(8)	1059(8)	197(5)
C(33)	7107(17)	5865(13)	440(10)	275(10)
C(34)	6785(12)	5641(12)	-81(11)	286(10)
C(35)	7572(6)	4296(5)	2770(5)	119(3)
C(36)	6381(7)	4533(6)	2989(6)	152(3)
C(37)	6039(8)	3679(7)	3263(7)	182(4)
C(38)	4907(10)	3898(9)	3470(9)	261(7)
C(39)	7735(7)	5741(5)	3269(6)	147(3)
C(40)	8070(9)	5289(7)	4063(6)	202(5)
C(41)	8057(11)	5475(8)	5476(8)	228(6)
C(42)	7679(11)	5834(8)	4756(8)	211(5)
Cl(1)	-5209(2)	8725(2)	1083(2)	142(1)
Cl(2)	4139(2)	6674(2)	-929(2)	156(1)
Cl(3)	4752(2)	6804(2)	4069(2)	149(1)
Cl(4)	-4611(2)	8779(2)	6065(1)	152(1)
N(1)	-1785(4)	8077(3)	2918(4)	78(1)
N(2)	-1322(4)	7835(3)	1046(3)	85(2)
N(3)	451(4)	7436(4)	668(3)	90(2)
N(4)	1339(4)	7391(3)	2243(4)	83(2)
N(5)	877(4)	7397(3)	4137(3)	86(2)
N(6)	-895(4)	7788(3)	4515(3)	84(2)
N(7)	8015(6)	5105(5)	2552(4)	123(2)
O(1)	-369(3)	8519(3)	1653(3)	83(1)
O(2)	-156(3)	8466(3)	3359(3)	81(1)
C(43)	-32(5)	1187(4)	2404(4)	90(2)
C(44)	-834(5)	649(4)	2549(4)	97(2)
C(45)	-1910(5)	1287(5)	2582(6)	139(3)
C(46)	-2754(6)	809(6)	2740(6)	166(4)
C(47)	1348(5)	-29(5)	3040(5)	106(2)
C(48)	1183(6)	390(5)	3835(6)	128(3)
C(49)	1545(6)	-310(5)	4546(5)	124(3)
C(50)	2675(7)	-670(6)	4531(7)	188(5)
C(51)	1714(5)	1332(4)	2163(4)	95(2)
C(52)	2870(5)	949(5)	2000(5)	134(3)
C(53)	3364(7)	1743(7)	1827(7)	170(4)
C(54)	4464(10)	1405(9)	1591(8)	248(6)
C(55)	1380(5)	-10(4)	1577(5)	97(2)
C(56)	1168(6)	464(5)	762(5)	121(3)
C(57)	1518(7)	-197(5)	20(6)	134(3)

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C(58)	2613(7)	-578(6)	-174(6)	159(3)
N(8)	1098(4)	622(3)	2301(3)	86(2)
Cl(5)	9474(2)	6861(1)	9331(1)	126(1)
Cl(6)	233(2)	7088(1)	6045(1)	135(1)

TABLE S8. Bond lengths [Å] and angles [°] for **1**·2[(*n*-Bu)$_4$N$^+$·Cl$^-$].

C(1)-N(1)	1.384(7)	N(1)-C(1)-C(2)	129.3(6)	C(42)-C(41)-H(41A)	109.5
C(1)-C(2)	1.403(8)	N(1)-C(1)-C(6)	108.8(6)	C(42)-C(41)-H(41B)	109.5
C(1)-C(6)	1.408(8)	C(2)-C(1)-C(6)	121.8(7)	H(41A)-C(41)-H(41B)	109.5
C(2)-C(3)	1.370(8)	C(3)-C(2)-N(6)	119.3(6)	C(42)-C(41)-H(41C)	109.5
C(2)-N(6)	1.395(7)	C(3)-C(2)-C(1)	116.6(6)	H(41A)-C(41)-H(41C)	109.5
C(3)-C(4)	1.394(8)	N(6)-C(2)-C(1)	123.8(6)	H(41B)-C(41)-H(41C)	109.5
C(3)-H(3)	0.930	C(2)-C(3)-C(4)	121.1(6)	C(41)-C(42)-C(40)	117.0(12)
C(4)-C(5)	1.352(9)	C(2)-C(3)-H(3)	119.5	C(41)-C(42)-H(42A)	108.1
C(4)-Cl(4)	1.742(7)	C(4)-C(3)-H(3)	119.5	C(40)-C(42)-H(42A)	108.1
C(5)-C(6)	1.414(9)	C(5)-C(4)-C(3)	124.2(7)	C(41)-C(42)-H(42B)	108.1
C(5)-H(5)	0.930	C(5)-C(4)-Cl(4)	118.1(6)	C(40)-C(42)-H(42B)	108.1
C(6)-C(7)	1.444(9)	C(3)-C(4)-Cl(4)	117.7(7)	H(42A)-C(42)-H(42B)	107.3
C(7)-C(8)	1.383(8)	C(4)-C(5)-C(6)	116.0(7)	C(1)-N(1)-C(12)	108.3(5)
C(7)-C(12)	1.397(8)	C(4)-C(5)-H(5)	122.0	C(1)-N(1)-H(1)	125.9
C(8)-C(9)	1.365(9)	C(6)-C(5)-H(5)	122.0	C(12)-N(1)-H(1)	125.9
C(8)-H(8)	0.930	C(1)-C(6)-C(5)	120.4(7)	C(13)-N(2)-C(11)	127.1(5)
C(9)-C(10)	1.394(9)	C(1)-C(6)-C(7)	106.9(6)	C(13)-N(2)-H(2)	116.4
C(9)-Cl(1)	1.753(6)	C(5)-C(6)-C(7)	132.6(7)	C(11)-N(2)-H(2)	116.4
C(10)-C(11)	1.382(7)	C(8)-C(7)-C(12)	120.5(7)	C(13)-N(3)-C(15)	127.1(5)
C(10)-H(10)	0.930	C(8)-C(7)-C(6)	133.1(7)	C(13)-N(3)-H(3A)	116.5
C(11)-C(12)	1.406(8)	C(12)-C(7)-C(6)	106.4(6)	C(15)-N(3)-H(3A)	116.5
C(11)-N(2)	1.408(7)	C(9)-C(8)-C(7)	117.7(7)	C(14)-N(4)-C(25)	109.3(5)
C(12)-N(1)	1.390(7)	C(9)-C(8)-H(8)	121.1	C(14)-N(4)-H(4)	125.3
C(13)-O(1)	1.244(7)	C(7)-C(8)-H(8)	121.1	C(25)-N(4)-H(4)	125.3
C(13)-N(3)	1.364(7)	C(8)-C(9)-C(10)	122.9(6)	C(26)-N(5)-C(24)	126.4(6)
C(13)-N(2)	1.376(7)	C(8)-C(9)-Cl(1)	121.0(6)	C(26)-N(5)-H(5A)	116.8
C(14)-N(4)	1.361(7)	C(10)-C(9)-Cl(1)	116.1(7)	C(24)-N(5)-H(5A)	116.8
C(14)-C(19)	1.419(8)	C(11)-C(10)-C(9)	120.3(7)	C(26)-N(6)-C(2)	127.3(6)
C(14)-C(15)	1.428(8)	C(11)-C(10)-H(10)	119.9	C(26)-N(6)-H(6)	116.3
C(15)-C(16)	1.367(8)	C(9)-C(10)-H(10)	119.9	C(2)-N(6)-H(6)	116.3
C(15)-N(3)	1.403(7)	C(10)-C(11)-C(12)	117.1(6)	C(35)-N(7)-C(27)	107.5(6)
C(16)-C(17)	1.380(9)	C(10)-C(11)-N(2)	118.1(7)	C(35)-N(7)-C(31)	111.9(7)
C(16)-H(16)	0.930	C(12)-C(11)-N(2)	124.5(6)	C(27)-N(7)-C(31)	111.2(7)
C(17)-C(18)	1.385(9)	N(1)-C(12)-C(7)	109.6(6)	C(35)-N(7)-C(39)	111.3(6)
C(17)-Cl(2)	1.750(7)	N(1)-C(12)-C(11)	128.8(6)	C(27)-N(7)-C(39)	109.1(7)
C(18)-C(19)	1.394(9)	C(7)-C(12)-C(11)	121.5(6)	C(31)-N(7)-C(39)	105.9(7)
C(18)-H(18)	0.930	O(1)-C(13)-N(3)	124.2(6)	N(8)-C(43)-C(44)	116.5(5)
C(19)-C(20)	1.429(9)	O(1)-C(13)-N(2)	122.8(6)	N(8)-C(43)-H(43A)	108.2
C(20)-C(21)	1.403(8)	N(3)-C(13)-N(2)	113.0(6)	C(44)-C(43)-H(43A)	108.2
C(20)-C(25)	1.411(8)	N(4)-C(14)-C(19)	108.6(6)	N(8)-C(43)-H(43B)	108.2
C(21)-C(22)	1.353(9)	N(4)-C(14)-C(15)	130.0(6)	C(44)-C(43)-H(43B)	108.2
C(21)-H(21)	0.930	C(19)-C(14)-C(15)	121.3(7)	H(43A)-C(43)-H(43B)	107.3
C(22)-C(23)	1.399(9)	C(16)-C(15)-N(3)	119.3(7)	C(45)-C(44)-C(43)	110.9(5)
C(22)-Cl(3)	1.735(7)	C(16)-C(15)-C(14)	117.5(6)	C(45)-C(44)-H(44A)	109.5
C(23)-C(24)	1.382(8)	N(3)-C(15)-C(14)	122.8(6)	C(43)-C(44)-H(44A)	109.5
C(23)-H(23)	0.930	C(15)-C(16)-C(17)	121.7(7)	C(45)-C(44)-H(44B)	109.5

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C(24)-C(25)	1.389(8)	C(15)-C(16)-H(16)	119.1	C(43)-C(44)-H(44B)	109.5
C(24)-N(5)	1.401(8)	C(17)-C(16)-H(16)	119.1	H(44A)-C(44)-H(44B)	108.0
C(25)-N(4)	1.398(7)	C(16)-C(17)-C(18)	121.5(7)	C(44)-C(45)-C(46)	114.2(7)
C(26)-O(2)	1.228(7)	C(16)-C(17)-Cl(2)	117.5(7)	C(44)-C(45)-H(45A)	108.7
C(26)-N(5)	1.365(7)	C(18)-C(17)-Cl(2)	121.0(7)	C(46)-C(45)-H(45A)	108.7
C(26)-N(6)	1.365(8)	C(17)-C(18)-C(19)	119.7(7)	C(44)-C(45)-H(45B)	108.7
C(27)-C(28)	1.507(12)	C(17)-C(18)-H(18)	120.1	C(46)-C(45)-H(45B)	108.7
C(27)-N(7)	1.513(9)	C(19)-C(18)-H(18)	120.1	H(45A)-C(45)-H(45B)	107.6
C(27)-H(27A)	0.970	C(18)-C(19)-C(14)	118.3(8)	C(45)-C(46)-H(46A)	109.5
C(27)-H(27B)	0.970	C(18)-C(19)-C(20)	134.4(7)	C(45)-C(46)-H(46B)	109.5
C(28)-C(29)	1.567(18)	C(14)-C(19)-C(20)	107.2(6)	H(46A)-C(46)-H(46B)	109.5
C(28)-H(28A)	0.970	C(21)-C(20)-C(25)	119.7(7)	C(45)-C(46)-H(46C)	109.5
C(28)-H(28B)	0.970	C(21)-C(20)-C(19)	133.7(7)	H(46A)-C(46)-H(46C)	109.5
C(29)-C(30)	1.128(16)	C(25)-C(20)-C(19)	106.5(6)	H(46B)-C(46)-H(46C)	109.5
C(29)-H(29A)	0.970	C(22)-C(21)-C(20)	117.4(7)	C(48)-C(47)-N(8)	117.2(6)
C(29)-H(29B)	0.970	C(22)-C(21)-H(21)	121.3	C(48)-C(47)-H(47A)	108.0
C(30)-H(30A)	0.960	C(20)-C(21)-H(21)	121.3	N(8)-C(47)-H(47A)	108.0
C(30)-H(30B)	0.960	C(21)-C(22)-C(23)	123.0(7)	C(48)-C(47)-H(47B)	108.0
C(30)-H(30C)	0.960	C(21)-C(22)-Cl(3)	119.0(7)	N(8)-C(47)-H(47B)	108.0
C(31)-N(7)	1.514(10)	C(23)-C(22)-Cl(3)	117.9(7)	H(47A)-C(47)-H(47B)	107.2
C(31)-C(32)	1.538(12)	C(24)-C(23)-C(22)	120.9(7)	C(47)-C(48)-C(49)	114.3(7)
C(31)-H(31A)	0.970	C(24)-C(23)-H(23)	119.6	C(47)-C(48)-H(48A)	108.7
C(31)-H(31B)	0.970	C(22)-C(23)-H(23)	119.6	C(49)-C(48)-H(48A)	108.7
C(32)-C(33)	1.545(17)	C(23)-C(24)-C(25)	116.8(7)	C(47)-C(48)-H(48B)	108.7
C(32)-H(32A)	0.970	C(23)-C(24)-N(5)	118.3(7)	C(49)-C(48)-H(48B)	108.7
C(32)-H(32B)	0.970	C(25)-C(24)-N(5)	124.6(6)	H(48A)-C(48)-H(48B)	107.6
C(33)-C(34)	1.160(18)	C(24)-C(25)-N(4)	129.4(6)	C(50)-C(49)-C(48)	116.8(8)
C(33)-H(33A)	0.970	C(24)-C(25)-C(20)	122.2(7)	C(50)-C(49)-H(49A)	108.1
C(33)-H(33B)	0.970	N(4)-C(25)-C(20)	108.3(7)	C(48)-C(49)-H(49A)	108.1
C(34)-H(34A)	0.960	O(2)-C(26)-N(5)	123.1(7)	C(50)-C(49)-H(49B)	108.1
C(34)-H(34B)	0.960	O(2)-C(26)-N(6)	123.3(7)	C(48)-C(49)-H(49B)	108.1
C(34)-H(34C)	0.960	N(5)-C(26)-N(6)	113.5(7)	H(49A)-C(49)-H(49B)	107.3
C(35)-N(7)	1.507(8)	C(28)-C(27)-N(7)	119.4(8)	C(49)-C(50)-H(50A)	109.5
C(35)-C(36)	1.532(9)	C(28)-C(27)-H(27A)	107.5	C(49)-C(50)-H(50B)	109.5
C(35)-H(35A)	0.970	N(7)-C(27)-H(27A)	107.5	H(50A)-C(50)-H(50B)	109.5
C(35)-H(35B)	0.970	C(28)-C(27)-H(27B)	107.5	C(49)-C(50)-H(50C)	109.5
C(36)-C(37)	1.505(11)	N(7)-C(27)-H(27B)	107.5	H(50A)-C(50)-H(50C)	109.5
C(36)-H(36A)	0.970	H(27A)-C(27)-H(27B)	107.0	H(50B)-C(50)-H(50C)	109.5
C(36)-H(36B)	0.970	C(27)-C(28)-C(29)	109.2(11)	C(52)-C(51)-N(8)	115.9(5)
C(37)-C(38)	1.458(12)	C(27)-C(28)-H(28A)	109.8	C(52)-C(51)-H(51A)	108.3
C(37)-H(37A)	0.970	C(29)-C(28)-H(28A)	109.8	N(8)-C(51)-H(51A)	108.3
C(37)-H(37B)	0.970	C(27)-C(28)-H(28B)	109.8	C(52)-C(51)-H(51B)	108.3
C(38)-H(38A)	0.960	C(29)-C(28)-H(28B)	109.8	N(8)-C(51)-H(51B)	108.3
C(38)-H(38B)	0.960	H(28A)-C(28)-H(28B)	108.3	H(51A)-C(51)-H(51B)	107.4
C(38)-H(38C)	0.960	C(30)-C(29)-C(28)	126.6(18)	C(51)-C(52)-C(53)	109.4(6)
C(39)-C(40)	1.507(11)	C(30)-C(29)-H(29A)	105.7	C(51)-C(52)-H(52A)	109.8
C(39)-N(7)	1.521(9)	C(28)-C(29)-H(29A)	105.7	C(53)-C(52)-H(52A)	109.8
C(39)-H(39A)	0.970	C(30)-C(29)-H(29B)	105.7	C(51)-C(52)-H(52B)	109.8
C(39)-H(39B)	0.970	C(28)-C(29)-H(29B)	105.7	C(53)-C(52)-H(52B)	109.8
C(40)-C(42)	1.402(12)	H(29A)-C(29)-H(29B)	106.1	H(52A)-C(52)-H(52B)	108.2
C(40)-H(40A)	0.970	C(29)-C(30)-H(30A)	109.5	C(54)-C(53)-C(52)	111.0(9)
C(40)-H(40B)	0.970	C(29)-C(30)-H(30B)	109.5	C(54)-C(53)-H(53A)	109.4
C(41)-C(42)	1.388(12)	H(30A)-C(30)-H(30B)	109.5	C(52)-C(53)-H(53A)	109.4

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C(41)-H(41A)	0.960	C(29)-C(30)-H(30C)	109.5	C(54)-C(53)-H(53B)	109.4
C(41)-H(41B)	0.960	H(30A)-C(30)-H(30C)	109.5	C(52)-C(53)-H(53B)	109.4
C(41)-H(41C)	0.960	H(30B)-C(30)-H(30C)	109.5	H(53A)-C(53)-H(53B)	108.0
C(42)-H(42A)	0.970	N(7)-C(31)-C(32)	115.1(7)	C(53)-C(54)-H(54A)	109.5
C(42)-H(42B)	0.970	N(7)-C(31)-H(31A)	108.5	C(53)-C(54)-H(54B)	109.5
N(1)-H(1)	0.860	C(32)-C(31)-H(31A)	108.5	H(54A)-C(54)-H(54B)	109.5
N(2)-H(2)	0.860	N(7)-C(31)-H(31B)	108.5	C(53)-C(54)-H(54C)	109.5
N(3)-H(3A)	0.860	C(32)-C(31)-H(31B)	108.5	H(54A)-C(54)-H(54C)	109.5
N(4)-H(4)	0.860	H(31A)-C(31)-H(31B)	107.5	H(54B)-C(54)-H(54C)	109.5
N(5)-H(5A)	0.860	C(31)-C(32)-C(33)	108.0(11)	C(56)-C(55)-N(8)	115.6(6)
N(6)-H(6)	0.860	C(31)-C(32)-H(32A)	110.1	C(56)-C(55)-H(55A)	108.4
C(43)-N(8)	1.509(7)	C(33)-C(32)-H(32A)	110.1	N(8)-C(55)-H(55A)	108.4
C(43)-C(44)	1.521(7)	C(31)-C(32)-H(32B)	110.1	C(56)-C(55)-H(55B)	108.4
C(43)-H(43A)	0.970	C(33)-C(32)-H(32B)	110.1	N(8)-C(55)-H(55B)	108.4
C(43)-H(43B)	0.970	H(32A)-C(32)-H(32B)	108.4	H(55A)-C(55)-H(55B)	107.4
C(44)-C(45)	1.491(8)	C(34)-C(33)-C(32)	124(2)	C(55)-C(56)-C(57)	114.5(7)
C(44)-H(44A)	0.970	C(34)-C(33)-H(33A)	106.4	C(55)-C(56)-H(56A)	108.6
C(44)-H(44B)	0.970	C(32)-C(33)-H(33A)	106.4	C(57)-C(56)-H(56A)	108.6
C(45)-C(46)	1.505(9)	C(34)-C(33)-H(33B)	106.4	C(55)-C(56)-H(56B)	108.6
C(45)-H(45A)	0.970	C(32)-C(33)-H(33B)	106.4	C(57)-C(56)-H(56B)	108.6
C(45)-H(45B)	0.970	H(33A)-C(33)-H(33B)	106.4	H(56A)-C(56)-H(56B)	107.6
C(46)-H(46A)	0.960	C(33)-C(34)-H(34A)	109.5	C(58)-C(57)-C(56)	113.0(7)
C(46)-H(46B)	0.960	C(33)-C(34)-H(34B)	109.5	C(58)-C(57)-H(57A)	109.0
C(46)-H(46C)	0.960	H(34A)-C(34)-H(34B)	109.5	C(56)-C(57)-H(57A)	109.0
C(47)-C(48)	1.465(9)	C(33)-C(34)-H(34C)	109.5	C(58)-C(57)-H(57B)	109.0
C(47)-N(8)	1.520(8)	H(34A)-C(34)-H(34C)	109.5	C(56)-C(57)-H(57B)	109.0
C(47)-H(47A)	0.970	H(34B)-C(34)-H(34C)	109.5	H(57A)-C(57)-H(57B)	107.8
C(47)-H(47B)	0.970	N(7)-C(35)-C(36)	116.1(6)	C(57)-C(58)-H(58A)	109.5
C(48)-C(49)	1.556(10)	N(7)-C(35)-H(35A)	108.3	C(57)-C(58)-H(58B)	109.5
C(48)-H(48A)	0.970	C(36)-C(35)-H(35A)	108.3	H(58A)-C(58)-H(58B)	109.5
C(48)-H(48B)	0.970	N(7)-C(35)-H(35B)	108.3	C(57)-C(58)-H(58C)	109.5
C(49)-C(50)	1.470(10)	C(36)-C(35)-H(35B)	108.3	H(58A)-C(58)-H(58C)	109.5
C(49)-H(49A)	0.970	H(35A)-C(35)-H(35B)	107.4	H(58B)-C(58)-H(58C)	109.5
C(49)-H(49B)	0.970	C(37)-C(36)-C(35)	111.1(7)	C(43)-N(8)-C(47)	112.9(5)
C(50)-H(50A)	0.960	C(37)-C(36)-H(36A)	109.4	C(43)-N(8)-C(55)	110.9(5)
C(50)-H(50B)	0.960	C(35)-C(36)-H(36A)	109.4	C(47)-N(8)-C(55)	104.6(5)
C(50)-H(50C)	0.960	C(37)-C(36)-H(36B)	109.4	C(43)-N(8)-C(51)	105.1(4)
C(51)-C(52)	1.489(8)	C(35)-C(36)-H(36B)	109.4	C(47)-N(8)-C(51)	111.7(5)
C(51)-N(8)	1.528(7)	H(36A)-C(36)-H(36B)	108.0	C(55)-N(8)-C(51)	111.9(5)
C(51)-H(51A)	0.970	C(38)-C(37)-C(36)	111.4(9)		
C(51)-H(51B)	0.970	C(38)-C(37)-H(37A)	109.3		
C(52)-C(53)	1.525(10)	C(36)-C(37)-H(37A)	109.3		
C(52)-H(52A)	0.970	C(38)-C(37)-H(37B)	109.3		
C(52)-H(52B)	0.970	C(36)-C(37)-H(37B)	109.3		
C(53)-C(54)	1.421(13)	H(37A)-C(37)-H(37B)	108.0		
C(53)-H(53A)	0.970	C(37)-C(38)-H(38A)	109.5		
C(53)-H(53B)	0.970	C(37)-C(38)-H(38B)	109.5		
C(54)-H(54A)	0.960	H(38A)-C(38)-H(38B)	109.5		
C(54)-H(54B)	0.960	C(37)-C(38)-H(38C)	109.5		
C(54)-H(54C)	0.960	H(38A)-C(38)-H(38C)	109.5		
C(55)-C(56)	1.502(9)	H(38B)-C(38)-H(38C)	109.5		
C(55)-N(8)	1.526(7)	C(40)-C(39)-N(7)	115.5(7)		
C(55)-H(55A)	0.970	C(40)-C(39)-H(39A)	108.4		

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C(55)-H(55B)	0.970	N(7)-C(39)-H(39A)	108.4		
C(56)-C(57)	1.571(9)	C(40)-C(39)-H(39B)	108.4		
C(56)-H(56A)	0.970	N(7)-C(39)-H(39B)	108.4		
C(56)-H(56B)	0.970	H(39A)-C(39)-H(39B)	107.5		
C(57)-C(58)	1.414(9)	C(42)-C(40)-C(39)	115.6(9)		
C(57)-H(57A)	0.970	C(42)-C(40)-H(40A)	108.4		
C(57)-H(57B)	0.970	C(39)-C(40)-H(40A)	108.4		
C(58)-H(58A)	0.960	C(42)-C(40)-H(40B)	108.4		
C(58)-H(58B)	0.960	C(39)-C(40)-H(40B)	108.4		
C(58)-H(58C)	0.960	H(40A)-C(40)-H(40B)	107.4		

TABLE S9. Anisotropic displacement parameters ($Å^2$ x 10^3) for **1**·2[(*n*-Bu)$_4$N$^+$·Cl$^-$]·2DMSO. The anisotropic displacement factor exponent takes the form $-2\pi^2$ [$h^2a^{*2}U^{11}$ + … $2hka^*b^*U^{12}$].

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	70(5)	67(4)	94(6)	-21(4)	-2(4)	-23(3)
C(2)	82(5)	77(4)	87(5)	-17(4)	-21(5)	-31(4)
C(3)	85(5)	92(5)	90(6)	-21(4)	-13(4)	-28(4)
C(4)	93(6)	110(5)	93(6)	-25(4)	4(5)	-38(4)
C(5)	80(5)	101(5)	114(7)	-21(5)	3(5)	-27(4)
C(6)	79(5)	83(4)	99(6)	-13(4)	-22(5)	-30(4)
C(7)	55(4)	80(4)	121(7)	-16(4)	-17(4)	-19(3)
C(8)	78(5)	101(5)	127(7)	-21(5)	-24(5)	-27(4)
C(9)	65(5)	101(5)	138(7)	-12(5)	-41(5)	-27(4)
C(10)	89(5)	84(5)	107(6)	2(4)	-39(5)	-29(4)
C(11)	64(4)	71(4)	104(6)	-14(4)	-15(4)	-21(3)
C(12)	75(5)	68(4)	90(5)	-10(4)	-20(4)	-23(3)
C(13)	81(5)	72(4)	83(5)	9(4)	-22(4)	-24(4)
C(14)	67(5)	76(4)	94(6)	-18(4)	-3(4)	-26(3)
C(15)	77(5)	69(4)	97(6)	-14(4)	-13(5)	-22(3)
C(16)	93(5)	92(5)	98(6)	-17(4)	-6(5)	-34(4)
C(17)	97(6)	110(6)	102(6)	-24(5)	14(5)	-38(4)
C(18)	77(5)	97(5)	143(8)	-23(5)	-11(6)	-35(4)
C(19)	62(5)	83(5)	118(7)	-24(4)	12(5)	-25(3)
C(20)	80(5)	79(4)	99(6)	-21(4)	-13(5)	-17(4)
C(21)	71(5)	105(5)	147(8)	-30(5)	-40(5)	-15(4)
C(22)	80(6)	107(6)	136(7)	-30(5)	-46(6)	-14(4)
C(23)	80(5)	86(5)	128(6)	-12(4)	-42(5)	-8(4)
C(24)	73(5)	72(4)	94(6)	-10(4)	-20(5)	-12(3)
C(25)	64(5)	76(4)	112(6)	-12(4)	-14(5)	-23(3)
C(26)	76(5)	75(5)	94(6)	-22(4)	-25(5)	-30(4)
C(27)	151(8)	102(6)	138(8)	-31(5)	-4(6)	-33(6)
C(28)	287(16)	187(11)	219(13)	-77(9)	68(12)	-145(12)
C(29)	184(13)	470(30)	310(20)	-230(20)	89(14)	-196(17)
C(30)	550(40)	320(20)	430(30)	-12(19)	-370(30)	-80(20)
C(31)	208(10)	106(7)	156(9)	2(7)	-41(8)	-35(6)
C(32)	273(14)	163(10)	170(11)	46(9)	-76(10)	-76(9)
C(33)	440(30)	299(19)	199(15)	84(14)	-159(16)	-230(20)
C(34)	182(12)	300(20)	340(30)	114(18)	-80(16)	-32(13)
C(35)	157(8)	71(5)	120(7)	1(4)	-14(5)	-30(5)
C(36)	119(7)	135(8)	177(9)	-23(7)	-3(6)	-9(6)
C(37)	151(9)	131(8)	252(13)	-28(8)	12(9)	-46(7)

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C(38)	187(13)	235(14)	360(20)	-38(13)	-7(13)	-73(11)
C(39)	173(8)	100(6)	144(8)	-51(6)	9(7)	-14(5)
C(40)	292(14)	146(9)	114(8)	-51(7)	-25(9)	27(9)
C(41)	338(19)	193(12)	161(12)	-45(10)	-67(12)	-63(11)
C(42)	291(16)	163(10)	173(12)	-42(10)	-39(12)	-45(10)
Cl(1)	99(1)	170(2)	170(2)	-21(2)	-60(1)	-33(1)
Cl(2)	120(2)	205(2)	145(2)	-51(2)	24(1)	-64(2)
Cl(3)	89(1)	176(2)	183(2)	-56(2)	-58(1)	-4(1)
Cl(4)	117(2)	199(2)	129(2)	-43(2)	23(1)	-46(2)
N(1)	61(3)	77(3)	97(4)	-18(3)	-20(3)	-11(2)
N(2)	82(4)	94(4)	91(4)	-14(3)	-30(3)	-32(3)
N(3)	79(4)	102(4)	97(4)	-28(3)	-13(3)	-32(3)
N(4)	63(3)	94(4)	100(5)	-14(3)	-17(4)	-27(3)
N(5)	80(4)	84(4)	96(4)	0(3)	-26(4)	-21(3)
N(6)	81(4)	91(4)	86(4)	1(3)	-22(3)	-31(3)
N(7)	146(6)	87(5)	119(6)	-6(4)	-9(5)	-13(4)
O(1)	85(3)	77(3)	94(3)	-14(2)	-24(2)	-28(2)
O(2)	81(3)	73(3)	98(3)	-7(3)	-23(3)	-28(2)
C(43)	83(5)	74(4)	110(5)	-21(4)	-12(4)	-17(4)
C(44)	76(5)	88(5)	129(6)	-17(4)	-18(4)	-23(4)
C(45)	83(5)	116(6)	210(10)	-29(6)	-10(5)	-21(5)
C(46)	89(6)	161(8)	245(12)	-17(7)	0(6)	-48(6)
C(47)	116(6)	94(5)	120(7)	3(5)	-27(5)	-49(4)
C(48)	149(7)	107(6)	143(8)	-16(6)	-23(6)	-56(5)
C(49)	138(7)	93(6)	143(8)	3(5)	-39(6)	-30(5)
C(50)	140(8)	132(8)	303(15)	-41(8)	-63(9)	-31(6)
C(51)	109(5)	83(5)	110(6)	1(4)	-20(4)	-54(4)
C(52)	94(6)	141(7)	185(9)	-13(6)	-1(5)	-73(5)
C(53)	104(7)	203(10)	231(11)	-1(8)	-18(7)	-95(7)
C(54)	245(15)	249(14)	299(17)	-5(12)	-22(13)	-160(13)
C(55)	93(5)	78(5)	119(6)	-18(5)	-4(4)	-27(4)
C(56)	135(6)	106(6)	123(7)	-40(6)	4(6)	-42(5)
C(57)	135(7)	97(6)	170(9)	-22(6)	-26(6)	-29(5)
C(58)	146(8)	131(8)	198(10)	-31(7)	-9(7)	-43(6)
N(8)	86(4)	71(3)	105(4)	-8(3)	-13(3)	-31(3)
Cl(5)	146(2)	119(2)	120(2)	-39(1)	-41(1)	-25(1)
Cl(6)	173(2)	109(2)	99(2)	-22(1)	-36(1)	9(1)

TABLE S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **1**·2[(*n*-Bu)$_4$N$^+$·Cl$^-$]·2DMSO. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
H(3)	-2462	8228	5671	105
H(5)	-4855	8841	4435	120
H(8)	-5040	8822	2752	120
H(10)	-3091	8290	586	108
H(16)	2009	7140	-502	112
H(18)	4365	6762	730	125
H(21)	4590	6822	2421	127
H(23)	2625	7123	4587	117
H(27A)	9420	4351	2823	158
H(27B)	9345	4302	1901	158

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H(28A)	9662	5844	2508	270
H(28B)	9720	5684	1573	270
H(29A)	11053	4174	2025	366
H(29B)	11364	4983	1497	366
H(30A)	11150	5124	2972	602
H(30B)	12030	5184	2220	602
H(30C)	11951	4216	2607	602
H(31A)	7933	6178	1697	190
H(31B)	6848	6004	2024	190
H(32A)	7404	4662	1196	237
H(32B)	8427	4941	820	237
H(33A)	6517	6288	767	330
H(33B)	7568	6226	174	330
H(34A)	7323	5165	-383	429
H(34B)	6560	6164	-447	429
H(34C)	6205	5409	156	429
H(35A)	7864	3949	3235	142
H(35B)	7805	3893	2308	142
H(36A)	6130	4968	3427	183
H(36B)	6078	4825	2511	183
H(37A)	6293	3243	2825	218
H(37B)	6342	3387	3740	218
H(38A)	4657	4312	3917	392
H(38B)	4712	3340	3632	392
H(38C)	4605	4188	2998	392
H(39A)	8049	6241	3106	176
H(39B)	6985	6012	3374	176
H(40A)	7854	4729	4178	243
H(40B)	8826	5108	3982	243
H(41A)	7844	4930	5666	341
H(41B)	7783	5928	5891	341
H(41C)	8804	5318	5371	341
H(42A)	7826	6424	4615	253
H(42B)	6927	5957	4870	253
H(1)	-1118	7888	2778	94
H(2)	-1286	7512	636	101
H(3A)	333	7137	299	108
H(4)	676	7491	2387	100
H(5A)	871	7086	4601	103
H(6)	-752	7450	4949	101
H(43A)	-132	1586	1913	108
H(43B)	-176	1583	2864	108
H(44A)	-684	227	2108	116
H(44B)	-789	286	3064	116
H(45A)	-1947	1643	2063	166
H(45B)	-2042	1718	3014	166
H(46A)	-2741	472	3263	249
H(46B)	-2637	388	2311	249
H(46C)	-3420	1261	2748	249
H(47A)	930	-456	3102	127
H(47B)	2074	-391	2916	127
H(48A)	446	703	3992	154
H(48B)	1555	854	3769	154

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H(49A)	1228	-13	5065	149
H(49B)	1273	-831	4540	149
H(50A)	2947	-173	4600	282
H(50B)	3008	-944	4012	282
H(50C)	2807	-1129	4970	282
H(51A)	1506	1743	1700	114
H(51B)	1518	1702	2646	114
H(52A)	3084	559	1529	161
H(52B)	3102	575	2475	161
H(53A)	3074	2152	1390	204
H(53B)	3201	2097	2318	204
H(54A)	4626	1029	1122	373
H(54B)	4758	1042	2040	373
H(54C)	4752	1917	1450	373
H(55A)	2116	-342	1518	117
H(55B)	995	-464	1709	117
H(56A)	1525	939	639	145
H(56B)	426	768	809	145
H(57A)	1198	-697	154	160
H(57B)	1267	145	-462	160
H(58A)	2857	-976	278	239
H(58B)	2938	-88	-270	239
H(58C)	2786	-928	-661	239

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